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FINAL REPORT

Efficient Load Balance and Locality of Reference for Unstructured Grid and Particle Simulations on Massively Parallel Processors

Contract F49620-93-1-0480

July 1, 1993 – November 30, 1995.

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1 Summary

During the contract period our main results are a computer code for fast parallel algorithms for particle systems interacting with long–range forces, analysis of the error characteristics of the chosen method, and a parallel implementation of a $O(N \log_2^2 N)$ algorithm for Legendre and Spherical transforms. We have also derived an algebraic framework for describing permutations frequently used in scientific computation. The framework allows for a rigorous analysis of the communication requirements of parallel algorithms and is also very useful in address computations during compilation or in run–time systems. For efficient data motion, or remote references, we have also further validated the potential benefits of ROMM routing.

Fast N–body algorithms

In the first phase of our project we showed that Anderson's method [2], based on Poisson's formula, can be efficiently implemented in a high–level language on scalable parallel architectures [10, 11], such as Connection Machine Fortran (CMF) [21]. High Performance Fortran (HPF) [7] has adopted many of the features of CMF. We simulated particle systems with up to 100 million particles on CM–5 and CM–5E systems. The code was listed as an "impressive entry" in the 1994 Gordon Bell competition.

The parallel implementation allowed us to develop an improved understanding of the accuracy–computational effort trade–off for Anderson's hierarchical method. For three digits of accuracy the method is competitive with direct N–body solvers at about 8,700 particles for

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three–dimensional problems, while for six digits of accuracy the break–even point is at about 38,000 particles. These empirical results are based on comparisons with the direct $O(N^2)$ method for systems with up to 1 million particles.

Hierarchical algorithms are the only alternative for simulation of large scale particle systems with long range forces whether gravitational or Columbic. Large scale for astrophysical systems and for certain molecular dynamics simulations may involve hundreds of millions of particles. Proposed methods for large particle systems include the $O(N \log_2 N)$ method by Barnes and Hut [3] and further developed by Salmon et. al. [17, 18], and $O(N)$ methods by Rokhlin and Greengard [8] (Multi–pole expansions), Anderson [2] (Poisson's formula), and Brandt [4] (multi–grid).

Anderson's method like the multi–pole and multi–grid methods is an approximate technique. For all methods higher accuracy can be achieved at increased computational effort. Though the computational time is directly proportional to the number of particles, the constant of proportionality depends upon the desired accuracy. Rokhlin and Greengard has given error bounds as a function of the number of terms in the multi–pole expansion, but accurate error estimates, i.e., how many terms are needed for a given desired accuracy and how it depends upon the particle distribution is not well understood. Similarly, Anderson provides some insights into the error characteristics of his method, but no rigorous tight bounds.

In our empirical study we explored how the accuracy varies with the parameters of the method (radii of the spheres of integration, number of terms in the expansion, the order of the integration method (number of integration points), the depth of the near–field, and the depth of the hierarchy), the distribution of particles, and the impact of using supernodes [11, 24]. Our studies showed that for the evaluation of Columbic forces in three–dimensions, using near–fields of a depth equal to one box and a hierarchy depth that minimizes the number of floating–point operations give the best running time for any desired accuracy. Supernodes are not applicable for near–fields with a depth of a single box.

We also studied how small variations of particle distributions would affect the accuracy of the method. We focused on varying the distribution of particles within leaf–level boxes while keeping the number of particles per leaf–level box constant. Our studies showed that with particles clustered in a corner of a leaf–level box and six digits of accuracy, close to one digit additional accuracy was achieved if the particles instead were clustered at the center of the leaf–level box. For unsymmetrical distributions, we found that enlarging the outer spheres of integration, which intuitively should smooth the field to be integrated, did not improve the accuracy.

A report summarizing the above results is in preparation [9]. Implementation techniques and benchmark data are presented in [10, 11].

Fast transforms

We are in the proess of devising, implementing and analyzing parallel versions of polynomial Cosine Transforms and a fast Legendre Transform (FLT) recently discovered by Driscoll and Healy [5]. The Legendre Transform is the basic component of spherical harmonics, which are used extensively in many scientific applications, especially meteorology and environmental sciences. The FLT computes the Legendre Transform in $O(N \log^2 N)$ operations compared to $O(N^2)$ operations for the classical approach. Aside from round–off errors, the Driscoll–Healey FLT is exact, as opposed to the $O(N \log^2 N)$ FLT proposed by Alpert and Rokhlin [1], which is based on the multi–pole expansion technique.

Novel modifications of the Driscoll–Healey algorithm that have been made in the course of this work is replacing convolutions with Cosine Transforms. This has been joint work with Maslen [12]. Since the Discrete Cosine Transform (DCT) is the key building block in our parallel FLT, most of the effort has been dedicated to comparing the *Classical DCT* [15, 16, 20], which makes use of the Fast Fourier Transform as the main computational structure, and the *Polynomial DCT* [19]. Variations of both algorithms have been compared from the perspective of parallel arithmetic, memory and communication complexity, as well as load–balance. A report is in preparation.

Efficient multi–processor communication

We have demonstrated that a new routing technique, ROMM routing, is only marginally less efficient than Dimension–order routing when such routing is optimal, and two to four times faster when Dimension–order routing performs poorly. Similarly, ROMM routing is two to four times faster than fully randomized routing for many interesting permutations, and only marginally slower when fully randomized routing performs well. The technique and simulation results are documented in two conference papers [13, 14].

Three approaches to communication in multi–processor systems is through libraries, special compilers, or general routers, with each approach having its advantages and disadvantages. General purpose routers are clearly necessary in general purpose computing environments, but the performance is often not sufficiently good for critical applications. For such applications communications libraries are typically used. However, such libraries are quite expensive to produce for production environments in which machine sizes and data array sizes and shapes may vary considerably. With an average development cost in the range $100,000 – $150,000 per library function, very few can be developed for each system, both from a cost point of view and a time–to–market point of view. Compiled routing can considerably reduce the cost and development time for library functions, or replace library functions alltogether. A communication compiler was developed for the Connection Machine CM–2/200. This compiler did not generate code sufficiently efficient for common communication patterns to eliminate the need for hand–optimized code, but produced sufficently efficient code to warrant its use for many irregular communications instead of the general router. A communication compiler was also developed at CMU for the iWarp [6], for which is was used successfully in a restricted setting. One fundamental difficulty with compiled routing is its

limited ability to efficiently handle communication patterns not known until run–time. For arbitrary communication patterns, and in particular for patterns that are not known until run–time, efficient general routers are highly desirable.

We have devised and explored a new routing technique, ROMM (Randomized Oblivious Minimal Multi–phase) routing. The idea is to attempt to combine the best properties of minimal routing and randomized routing. Minimal algorithms are optimal for a number of important routing patterns on some networks (such as CSHIFT on meshes and binary cubes, bit–complement permutations and random permutations). However, the most popular minimal algorithm, Dimension–order routing, performs very poorly on permutations such as transposition and bit–reversal. Fully randomized algorithms, such as Valiant–Brebner routing [22, 23], may perform better than Dimension–order routing for permutations such as transpose and bit–reversal (asymptotically fully randomized algorithms are guaranteed to perform better), but usually performs relatively poorly on permutations where Dimension–order routing performs well.

ROMM provides a mechanism for controlling the amount of randomization introduced and limiting the resources required for deadlock freedom. The technique is straightforward and may be used for general–purpose routing algorithms in networks which use store–and–forward, virtual cut–through, or wormhole routing.

Using the ROMM framework, we have developed a method for defining and analyzing algorithms in the class, and defined ROMM algorithms for mesh, torus, and binary cube networks. Analytical results show that these algorithms have the potential to outperform deterministic, oblivious routing algorithms and fully–randomized routing algorithms for a variety of representative routing tasks. Using a parallel simulator, we have shown that for wormhole–routed mesh, torus, and binary cube networks with up to 1024 nodes, ROMM algorithms are competitive with Dimension–order routing, and in some cases, more than two times faster for two–dimensional square meshes with up to 1024 nodes and faster still for binary cube networks. Our results also show that ROMM algorithms are up to three times faster than Valiant–Brebner routing for many routing problems and that ROMM routing scales well to larger network sizes.

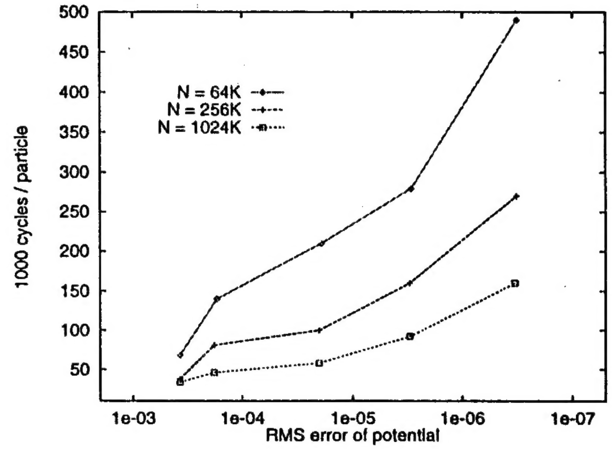
N-body Simulation of 100 Million Particles

Yu Hu and S. Lennart Johnsson
Harvard University

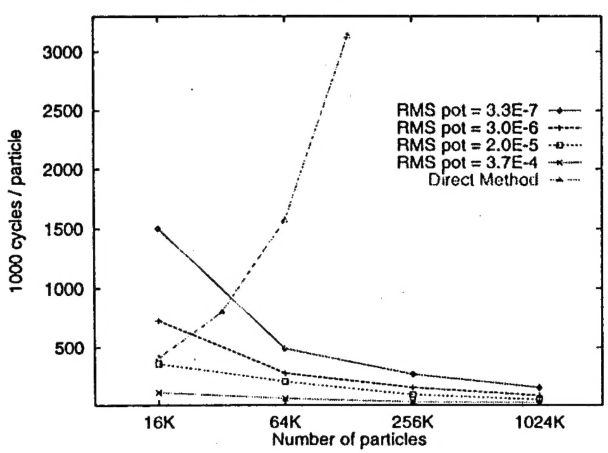
Siloxane structure
Courtesy of
Dr. Ruth Pachter, WPAFB
(Candidate application)

- 100M particle potential evaluation in 3 minutes on 256PN CM-5E, expected error decay rate 4, expected error 4E-04.
- 100M particle potential evaluation in 15 minutes on 256PN CM-5E, expected error decay rate 9, expected error 3E-07.

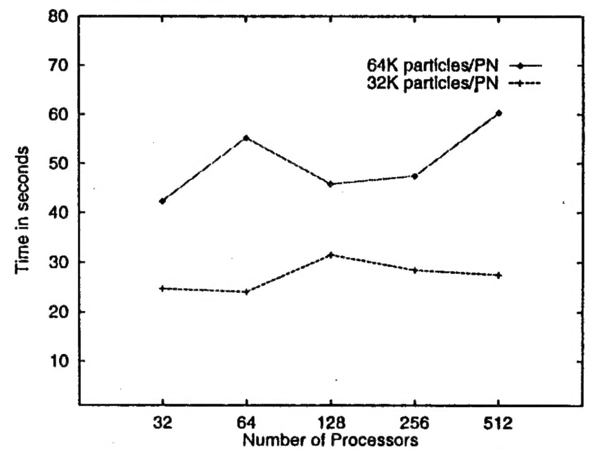
Cost vs. Accuracy (32PN CM-5E)



Efficiency (32PN CM-5E)

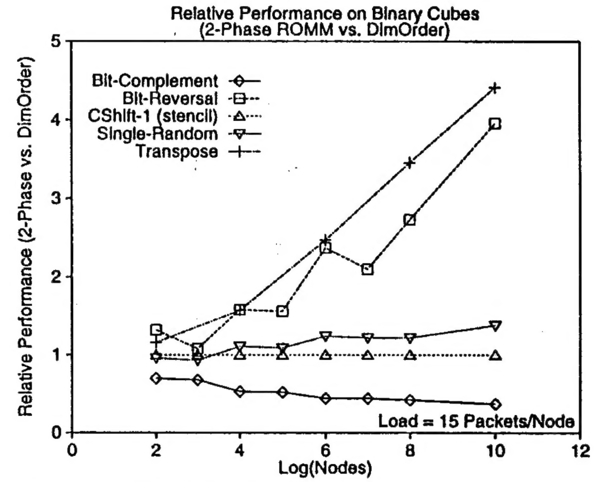


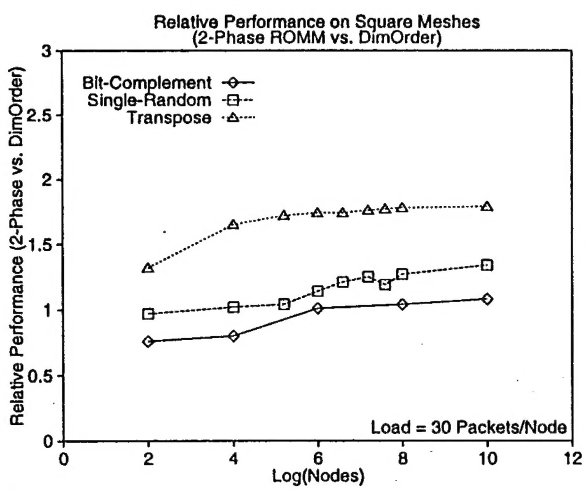
Scalability (CM-5)

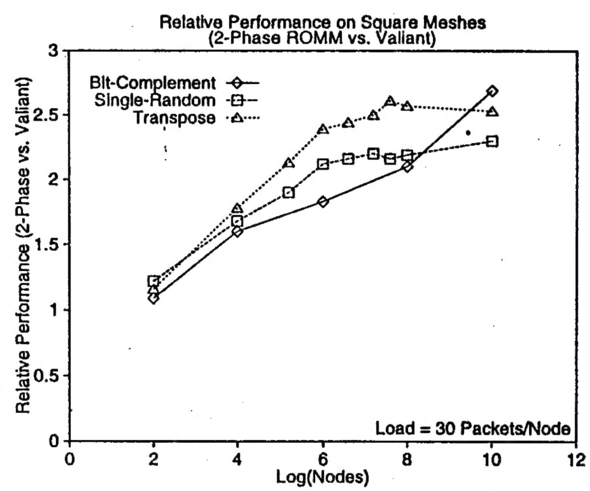


ROMM Routing

- Oblivious
- Minimal
- Controlled randomization
- Performance competitive with customized routing and worst–case optimal routing
- Modest hardware cost
- No special software required







Ted Nesson and S. Lennart Johnsson

Harvard University

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[10] Yu Hu and S. Lennart Johnsson. A data parallel implementation of hierarchical N–body methods. *International Journal of Supercomputer Applications*, 10(1), 1996. Also available as TR–26–94, Harvard University, Division of Applied Sciences, September, 1994.

[11] Yu Hu and S. Lennart Johnsson. Implementing $O(N)$ N–body algorithms efficiently in data parallel languages. *Journal of Scientific Programming*, 1996. Also available as TR–24–94, Harvard University, Division of Applied Sciences, September, 1994.

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[13] Ted Nesson and S. Lennart Johnsson. ROMM routing: A class of efficient minimal routing algorithms. In Kevin Bolding and Lawrence Snyder, editors, *Proceedings of the Parallel Computer Routing and Communication Workshop*, pages 185–199. Springer–Verlag, 1994. Lecture Notes in Computer Science, 853.

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[24] Feng Zhao. An O(N) algorithm for three–dimensional N–body simulations. Technical Report AI Memo 995, MIT, Artificial Intelligence Laboratory, October 1987.

2 Supported Ph.D. Students

1993 – present	Yu Hu: Harvard University.
	Nadia Shalaby: Harvard University.
1993 – 1995	Ted Nesson: Constrained randomization for routing in computer networks Harvard University.
	Dimitrios Kehagias: Harvard University.

3 Ph.D Thesis Committees

1992 –	Nikos K. Filippopoulos; Harvard University
1992 – 1994	Michel Jacquemin: Compiling for Distributed Memory Machines, Yale University.
	Pangfeng Liu: Efficient Parallel N–body simulation, Yale University.
	Chun–Hung Chen: An Efficient Approach for Discrete Event System Decision Problems, Harvard University.

4 Editorial Work

- 1991 – present:
  Editorial Board, International Journal of Supercomputer Applications.
- 1991 – present:
  Editorial Advisory Board, Journal of Scientific Programming.
- 1990 – present:
  Editorial Board, Journal for Numerical Linear Algebra with Applications.
- 1988 – present:
  Editorial Board, Journal on Concurrency: Practice and Experience.
- 1988 – present:
  Editor, International Journal on High Speed Computing.
- 1984 – present:
  Editor, Journal of Parallel and Distributed Computing.

5 Boards and Committees

Professional committees:

1994 –	Industrial Advisory Board, West Virginia Experimental Program to Stimulate Competitive Research
1993 –	Steering Committee, Conference series on *Massively Parallel Processing Using Optical Interconnections*
1992 – 1994	Board Member, Computing Research Association
1992 – 1994	Steering Committee, DIMACS Parallel Implementation Challenge.

Conference committees:

1995 – 1996	Program Committee, *Third International Conference on Massively Parallel Processing Using Optical Interconnections,* October 20 – 22, 1996, Maui, Hawaii.
1995 – 1996	Program Committee, *The 1996 International Conference on Parallel Processing*, August 12 – 16 1996.
1994 – 1995	Program Committee, *Second International Conference on Massively Parallel Processing Using Optimal Interconnections,* October 23 – 24 1995, San Antonio, Texas.
1994 – 1995	Program Committee, *Fifth Symposium on Principles and Practice of Parallel Programming*, PPoPP 95, Santa Barbara, July 19 – 21, 1995
1994 – 1995	Program Committee, *Nineth International Parallel Processing Symposium,* April 1995, Santa Barbara
1993 – 1994	Program Committee, *Eighth International Parallel Processing Symposium,* April 1994, Cancun, Mexico
1993 – 1994	Program Committee, *First International Workshop on Parallel Processing Using Optical Interconnect*, April, Cancun, Mexico, 1994.

Other committees:

1995 – present	Distinguished Professorships Committee, University of Houston

1995 – present Chair, Executive Committee, Department of Computer Science, University of Houston

1995 – present Chair, Faculty Search Committee, Department of Computer Science, University of Houston

1995 – present Chair, Chair Search Committee, Department of Computer Science, University of Houston

1995 – present Campus Computing Working Group, University of Houston

1993 Serge G. Petiton, L'Habilitation a Diriger des Recherches, Contribution a une Methodologie Globale Pour Le Calcul Scientifique Parallele, University of Paris VI.

6 Honors and Awards:

"Impressive Entry" recognition in the 1994 Gordon Bell Prize contest (with Yu Hu).

7 Journal Publications

"Local Basic Linear Algebra Subroutines (LBLAS) for the CM–5/5E", (with David Kramer and Yu Hu), to appear in the *International Journal of Supercomputer Applications*, vol. , no. , pp. , 1996.

"A Data Parallel Implementation of Hierarchical N–body Methods", (with Yu Hu), to appear in the *International Journal of Supercomputer Applications*, vol. , no. , pp. , 1996.

"Implementing $O(N)$ N–body algorithms efficiently in data parallel languages", (with Yu Hu), to appear in the *Journal of Scientific Programming*, vol. , no. , pp. , 1996.

"All–to–All Communication on the Connection Machine system CM–200", (with Kapil K. Mathur), the *Journal of Scientific Programming*, vol. 4, no. 4, pp. 251 – 273, 1995.

"On the Conversion between Binary Code and Binary Reflected Gray Code", (with Ching-Tien Ho), in *IEEE Transactions on Computers*, vol. 44, no. 1, pp. 47 – 53, January 1995.

"Index Transformation Algorithms in a Linear Algebra Framework", (with Alan Edelman and Steve Heller), in *Transactions on Parallel and Distributed Systems*, vol. 5, no. 12, pp. 1302 – 1309, 1994.

"Scalability of Finite Element Applications on Distributed–Memory Parallel Computers", (with Zdenek Johan and Kapil K. Mathur and S. Lennart Johnsson and Thomas J.R. Hughes), in *Computer Methods in Applied Mechanics and Engineering*, vol. 119, nos. 1 – 2, pp. 61 – 72, November 1994.

"Issues in High Performance Computer Networks", in *IEEE Technical Committee on Computer Architecture Newsletter*, Summer – Fall 1994, pp. 14 – 19.

"Optimal Communication Channel Utilization for Matrix Transposition and Related Permutations on Boolean Cubes", (with Ching–Tien Ho) in the *Journal of Discrete Applied Mathematics*, vol. 53, pp. 251 – 274, September 1994.

"Multiplication of Matrices of Arbitrary Shape on a Data Parallel Computer", (with Kapil K. Mathur), in *Journal of Parallel Computing*, vol. 20, no. 7, pp. 919 - 951, July, 1994.

"An Efficient Communication Strategy for Finite Element Methods on the Connection Machine CM–5 System", (with Zdenek Johan, Kapil K Mathur, and Thomas J.R. Hughes), in *Computer Methods in Applied Mechanics and Engineering*, vol. 113, pages 363 – 387, 1994.

"POLYSHIFT Communications Software for the Connection Machine System CM–200", (with Ralph Brickner and William George), *Journal of Scientific Programming*, vol. 3, no. 1, pp. 83 – 99, Spring 1994.

"Boolean Cube Emulation of Butterfly Networks Encoded by Gray Code" (with Ching–Tien Ho), *Journal of Parallel and Distributed Computing*, vol. 20, no. 3, pp 261 – 279, 1994.

"An Efficient Algorithm for Gray–to–Binary Permutation on Hypercubes", (with Ching–Tien Ho and M.T. Raghunath), *Journal of Parallel and Distributed Computing*, vol. 20, no. 1, pp. 114 – 120, 1994.

"Embedding Hyper–pyramids in Hypercubes", (with Ching–Tien Ho), *IBM Journal of Research and Development*, vol. 38, no. 1, pp. 31 – 45, 1994.

"Minimizing the Communication Time for Matrix Multiplication on Multiprocessors", *Journal of Parallel Computing*, vol. 19, no. 11, pp. 1235 – 1257, 1993.

"Block Cyclic Dense Linear Algebra", (with Woody Lichtenstein), *SIAM J. of Sci. Comp.*, vol. 14, no. 6, pp. 1257 – 1286, 1993.

8 Invited Presentations

1995

"Data Partitioning for Load–Balance and Communication Bandwidth Preservation", *The Second International Conference on Massively Parallel Processing and Optical Interconnections*, San Antonio, Texas, October 23 – 24, 1995.

"Structured Linear Algebra Software on Scalable Architectures", *International Congress on Industrial and Applied Mathematics*, Hamburg Germany, July 3 – 7, 1995.

"On the Accuracy of Fast N–body Algorithms", AFOSR PI–meeting, Phillips Laboratory, Kirtland Air Force Base, Albuquerque, New Mexico, June 28 – 30, 1995.

"A Stencil Compiler for the Connection Machine Model CM–5", *5th Workshop on Compilers*

for Parallel Computers, Malaga, Spain, June 28 – 30, 1995.

"Implementing O(N) N–body Algorithms Efficiently in Data Parallel Languages (High Performance Fortran)", Los Alamos National Laboratories, Los Alamos, New Mexico, June 15, 1995.

"On the Error in Anderson's Fast N–body Algorithm", The Royal Institute of Technology, May 30, 1995, Stockholm, Sweden.

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", Michigan State University, East Lansing, March 16 – 17, 1995.

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", the *Mardi Gras Conference on High Performance Computing Technologies*, Baton Rouge, Luisianna, February 23 - 25, 1995.

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", the Institute for Computer Science, Linköping University, Linköping, Sweden, January 10, 1995.

1994

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", the *Parallel Computation Center Annual Symposium*, the Royal Institute of Technology, Stockholm, Sweden, December 15 – 16, 1994.

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", Northwestern University, Evanston, Illinois, December 7, 1994.

"ROMM Routing: A Class of Efficient Minimal Rouitng Algorithms", Applied Mathematics Seminar series, California Institute of Technology, Pasadena, California, December 1, 1994.

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", Center for Research in Parallel Computation, California Institute of Technology, Pasadena, California, November 30, 1994.

"Scientific Supercomputing: Making MPP's deliver on their performance", *Computacion Cientifica en Paralelo*, Mexico City, Mexico, October 27 – 28, 1994.

"Implementing O(N) N-body algorithms efficiently in data parallel languages (High Performance Fortran)", *DIMACS Third Annual Implementation Challenge Workshop*, DIMACS, Rutgers University, New Brunswick, New Jersey, October 17 – 18, 1994.

"Scientific Supercomputing: Making MPP's deliver on their promise of high performance", *ICASE NASA Langley Industry Roundtable*, Williamsburgh, Virginia, October 3 – 4, 1994.

"Parallel Hierarchical N-Body Algorithms for Long Range Forces", AFOSR Workshop on *Large Scale Simulations in Chemistry/Material Science*, September 12 – 13, Dayton, Ohio, 1994.

"ROMM Routing: A Class of Efficient Minimal Routing Algorithms", NEC Research Institute, August 5, Princeton, New Jersey, 1994.

"Load–Balanced LU and QR Factor and Solve Routines for Scalable Processors with Scalable I/O", 14th IMACS World Congress, *Parallel Linear Algebra,* July 11 – 15, Atlanta, Georgia, 1994.

"High Performance Computing: Scalable Libraries, Scalable Applications", 14th IMACS World Congress, *Parallel Linear Algebra,* July 11 – 15, Atlanta, Georgia, 1994.

"Scalable Scientific Software Libraries", Workshop on *Parallel Scientific Computing,* UNI–C, Lyngby, Denmark, June 20 – 23, 1994.

"Scientific Supercomputing: Making MPPs deliver on their promise of high performance", the University of Houston, Houston, Texas, May 26, 1994.

"ROMM Routing: A Class of Efficient Minimal Routing Algorithms", *Parallel Computer Routing and Communication* Workshop, University of Washington, Seattle, Washington, May 16 – 18, 1994.

"Data Motion in High Performance Computing", First International Workshop on *Massively Parallel Processing Using Optical Interconnections,* Cancun, Mexico, April 26 – 27, 1994.

"Scientific Computation on Scalable Architectures", *TIMS ORSA Joint National Meeting,* Boston, Massachusetts, April 24 – 27, 1994.

"Data Parallel Finite Element Techniques for Compressible Flow Problems", (with Zdenek Johan, Kapil K. Mathur, and Thomas J.R. Hughes), *Proceedings of the Parallel Computational Fluid Dynamics 1994 Workshop,* Tokyo, March 1994.

"Performance of the Connection Machine System CM–5", *ARPA High Performance Computing and Communications Symposium*", Alexandria, Virginia, March 15 – 18 1994.

"Scientific Libraries on Scalable Architectures", Conference on *Teraflop Computing,* Baton Rouge, Louisianna, February 10 – 12, 1994.

"Locality in High Performance Parallel Computing", DIMACS Workshop on *Organizing and Moving Data in Parallel Computers,* Princeton, New Jersey, January 26 – 28, 1994.

"The Connection Machine System CM–5", the University of Tennessee, Tennessee, January 19, 1994.

1993

"Scientific Libraries on Scalable Architectures", Workshop on *Parallel Scientific Computation,* Stockholm, Sweden, December 15 – 17, 1993.

"A Stencil Compiler for the Connection Machine Models CM–2/200", Fourth International Workshop on *Compilers for Parallel Computers,* Delft, The Netherlands, December 13–16, 1993.

"Scientific Libraries on Scalable Architectures", Cornell University, Ithaca, New York, November 29, 1993.

"Scientific Libraries on Scalable Architectures", University of Maryland, College Park, Maryland, November 18, 1993.

"Scientific Libraries on Scalable Architectures", Bellcore, Morristown, New Jersey, November 9, 1993.

"Scientific Libraries on Scalable Architectures", Los Alamos National Laboratories, Los Alamos, New Mexico, October 29, 1993.

"Scalability of Finite Element Applications on Distributed–Memory Parallel Computers", (with Zdenek Johan and Kapil K. Mathur and S. Lennart Johnsson and Thomas J.R. Hughes), Presented at the *Symposium on Parallel Finite Element Computations*, Minneapolis, Minnesota, October, 1993.

"Scientific Libraries on Scalable Architectures", CERN, Geneva, Switzerland, October 14, 1993.

"The CMSSL", *Second European Connection Machine Users Group Conference*, Paris, France, October 13, 1993.

"Scientific Libraries on Scalable Architectures", *Scalable Parallel Libraries Conference*, Mississippi State University, Starkville, Mississippi, October 6 – 8, 1993.

"Scientific Libraries on Scalable Architectures", ARPA HPCC Semiannual meeting, San Diego, California, September 28 – 29, 1993.

"Finite Element Techniques for Computational Fluid Dynamics on the Connection Machine CM–5 System", with Z. Johan, K.K. Mathur, S.L. Johnsson and T.J.R. Hughes, the *Second US Congress on Computational Mechanics*, Washington D.C., August 1993.

"Scientific Libraries on Scalable Architectures", Workshop on *Portability and Performance for Parallel Processing*, Southampton, Hampshire, England, July 13 – 15, 1993.

"The Connection Machine System CM–5", *SPAA–93*, Sport Schloss Velen, Germany, June 30 – July 2, 1993.

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